EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	26	(546/269.4).CCLS.	US-PGPUB	OR	OFF	2007/09/20 11:48

=> file casreact
FILE 'CASREACT' ENTERED AT 10:57:25 ON 20 SEP 2007

FILE CONTENT:1840 - 15 Sep 2007 VOL 147 ISS 13

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****
*
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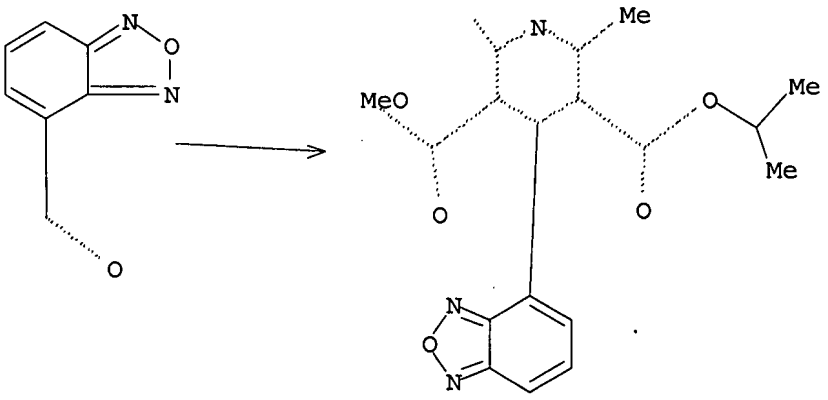
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 1 SEA FILE=CASREACT SSS FUL L1 (1 REACTIONS)

=> d l3 ibib abs fcrd

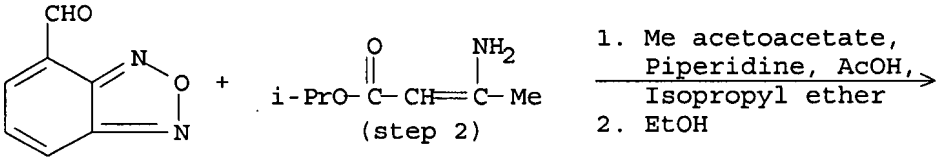
L3 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 142:155958 CASREACT
TITLE: Process for the manufacture of isradipine from the condensation reaction of 2,1,3-benzoxadiazole-4-carboxaldehyde and methyl acetoacetate and cyclocondensation of the intermediate with isopropyl β-aminocrotonate
INVENTOR(S): Thakashinamoorthy, Chandiran; Senthil, Kumar Minor; Palanivel, Kaliyaperumal; Mullaiyur, Radhakrishnan Selvaraju

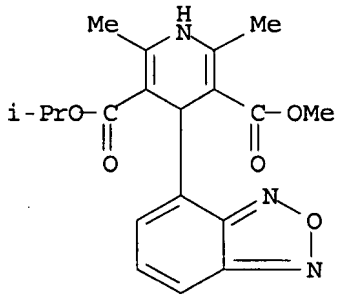
PATENT ASSIGNEE(S): Shasun Chemicals and Drugs Limited, India
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005005437	A1	20050120	WO 2004-IN208	20040715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN 2003CH00571	A	20070504	IN 2003-CH571	20030715
US 2006167063	A1	20060727	US 2006-564804	20060113
PRIORITY APPLN. INFO.:			IN 2003-CH571	20030715
			WO 2004-IN208	20040715

AB Isradipine, 4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid Me 1-methylethyl ester (I), is prepared in high yield and selectivity by reacting 2,1,3-benzoxadiazole-4-carboxaldehyde with Me acetoacetate in the presence of acetic acid and piperidine in diisopropyl ether to obtain 2-acetyl-3-benzofurazan-4-ylacrylic acid Me ester which is purified and then reacted with iso-Pr β-aminocrotonate in ethanol at 25-35° to give I.

RX(3) OF 3 - 2 STEPS





67%

CON: STEP(1.1) room temperature; 70 deg C
STEP(2.1) room temperature; 5 hours, 25 - 28 deg C

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> => file caplus
FILE 'CAPLUS' ENTERED AT 10:59:08 ON 20 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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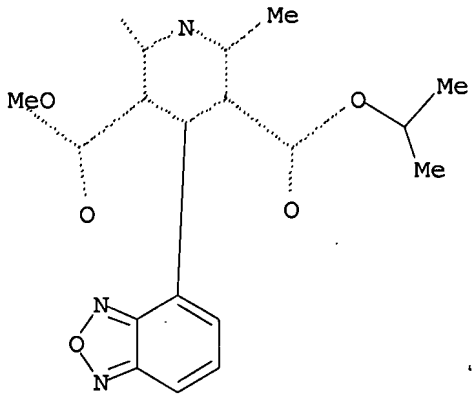
FILE COVERS 1907 - 20 Sep 2007 VOL 147 ISS 13
FILE LAST UPDATED: 19 Sep 2007 (20070919/ED)

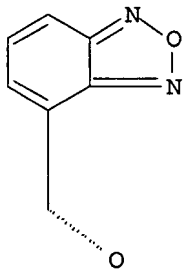
Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> d que
L4 STR



Structure attributes must be viewed using STN Express query preparation.
L5 STR



Structure attributes must be viewed using STN Express query preparation.
L6 31 SEA FILE=REGISTRY SSS FUL L4

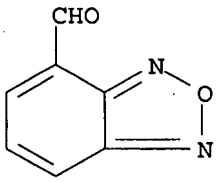
L7 42 SEA FILE=REGISTRY SSS FUL L5
L9 8 SEA FILE=CAPLUS L6 AND L7

=> d l9 1-8 ibib abs hitstr

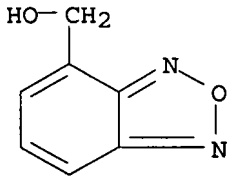
L9 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:238972 CAPLUS
DOCUMENT NUMBER: 142:316844
TITLE: Process for the manufacture of 2,1,3-benzoxadiazole-4-carboxaldehyde
INVENTOR(S): Chandiran, Thakashina Moorty; Subramaniam, S. S.; Swaminathan, Venkatraman
PATENT ASSIGNEE(S): Shasun Chemicals and Drugs Limited, India
SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023787	A1	20050317	WO 2003-IN305	20030910
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003269482	A1	20050329	AU 2003-269482	20030910
IN 2005CN02579	A	20070720	IN 2005-CN2579	20051010
IN 2005CN03165	A	20070727	IN 2005-CN3165	20051128
PRIORITY APPLN. INFO.:			WO 2003-IN305 A	20030910

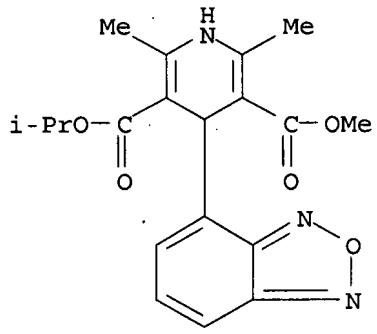
OTHER SOURCE(S): CASREACT 142:316844
AB A process is disclosed for the manufacture of 2,1,3-benzoxadiazole-4-carboxaldehyde, an intermediate for the preparation of 4-(4-Benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid Me 1-methylethyl ester (Isradipine). For instance, 2,1,3-benzoxadiazole-4-yl-methanol is oxidized to 2,1,3-benzoxadiazole-4-carboxaldehyde using pyridinium chlorochromate (PCC) in CH2Cl2 (0° (during addition of carbinol) -> 25-30°, 2 h) in 51% yield with 98.2% purity by HPLC (after silica gel filtration). The current process is more amenable to large scale preparation than prior art methods.
IT 32863-32-4P, 2,1,3-Benzoxadiazole-4-carboxaldehyde
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for manufacture of 2,1,3-benzoxadiazole-4-carboxaldehyde)
RN 32863-32-4 CAPLUS
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



IT 175609-19-5, (2,1,3-Benzoxadiazole-4-yl)methanol
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for manufacture of 2,1,3-benzoxadiazole-4-carboxaldehyde)
RN 175609-19-5 CAPLUS
CN 2,1,3-Benzoxadiazole-4-methanol (CA INDEX NAME)



IT 75695-93-1, Isradipine
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(process for manufacture of 2,1,3-benzoxadiazole-4-carboxaldehyde)
RN 75695-93-1 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:58213 CAPLUS
DOCUMENT NUMBER: 142:155958
TITLE: Process for the manufacture of isradipine from the condensation reaction of 2,1,3-benzoxadiazole-4-carboxaldehyde and methyl acetoacetate and cyclocondensation of the intermediate with isopropyl β-aminocrotonate
INVENTOR(S): Thakashinamoorthy, Chandiran; Senthil, Kumar Minor; Palanivel, Kaliyaperumal; Mullaiyur, Radhakrishnan Selvaraju
PATENT ASSIGNEE(S): Shasun Chemicals and Drugs Limited, India
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005005437	A1	20050120	WO 2004-IN208	20040715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
IN 2003CH00571	A	20070504	IN 2003-CH571	20030715
US 2006167063	A1	20060727	US 2006-564804	20060113
PRIORITY APPLN. INFO.:			IN 2003-CH571 A	20030715
			WO 2004-IN208 W	20040715

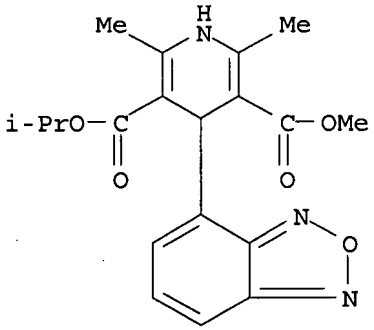
OTHER SOURCE(S): CASREACT 142:155958

AB Isradipine, 4-(4-benzofurazanyl)-1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylic acid Me 1-methylethyl ester (I), is prepared in high yield and selectivity by reacting 2,1,3-benzoxadiazole-4-carboxaldehyde with Me acetoacetate in the presence of acetic acid and piperidine in diisopropyl ether to obtain 2-acetyl-3-benzofurazan-4-ylacrylic acid Me ester which is purified and then reacted with iso-Pr β-aminocrotonate in ethanol at 25-35° to give I.

IT 75695-93-1P, Isradipine
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the manufacture of isradipine from the condensation reaction of 2,1,3-benzoxadiazole-4-carboxaldehyde and Me acetoacetate and cyclocondensation of the intermediate with iso-Pr β-aminocrotonate)

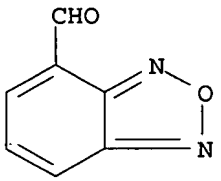
RN 75695-93-1 CAPLUS

CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)



IT 32863-32-4, 2,1,3-Benzoxadiazole-4-carboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the manufacture of isradipine from the condensation reaction of 2,1,3-benzoxadiazole-4-carboxaldehyde and Me acetoacetate and cyclocondensation of the intermediate with iso-Pr β-aminocrotonate)

RN 32863-32-4 CAPLUS
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)

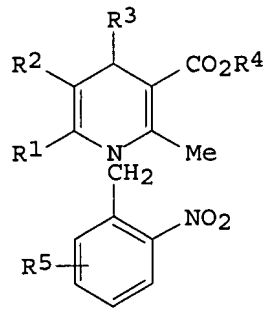


REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:217302 CAPLUS
DOCUMENT NUMBER: 120:217302
TITLE: Preparation of 1-(2-nitrobenzyl)-1,4-dihydropyridinecarboxylates as light-activated prodrugs for calcium modulators
INVENTOR(S): Goldmann, Siegfried; Bechem, Martin
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
DE 4222770	A1	19940113	DE 1992-4222770		19920710
WO 9401405	A1	19940120	WO 1993-EP1720		19930703
W: JP, US					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
EP 650477	A1	19950503	EP 1993-915785		19930703
R: DE, FR, GB					
US 5606066	A	19970225	US 1995-356410		19950501
PRIORITY APPLN. INFO.:			DE 1992-4222770	A	19920710
			WO 1993-EP1720	W	19930703

OTHER SOURCE(S): MARPAT 120:217302
GI



I

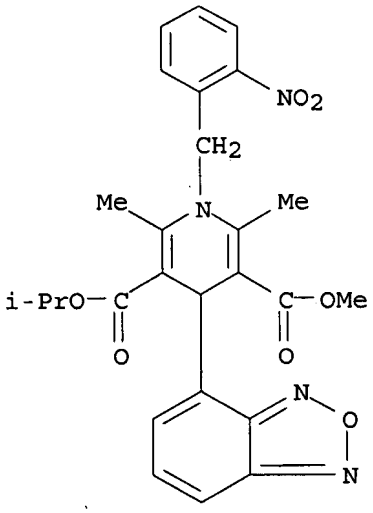
AB Title compds. [I; R1 = H, cyano, CHO, alkyl, etc.; R2 = cyano, NO2, alkoxycarbonyl, etc.; R1R2 = CH2O2C; R3 = aryl, heterocyclyl, etc.; R4 = (substituted)alk(en)yl; R5 = H, halo, OH, CO2H, etc.] were prepared Thus, 3-(O2N)C6H4CHO was cyclocondensed with MeCOCH2CO2Me and 2-(O2N)C6H4CH2NH2

to give I [R1 = R4 = Me, R2 = CO2Me, R3 = 3-(O2N)C6H4, R5 = H]. Contractile force tracings of perfused guinea pig papillary muscle under unirrad. and irrad. I treatment were given.

IT 154026-72-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as photoactivated calcium modulator prodrug)

RN 154026-72-9 CAPLUS

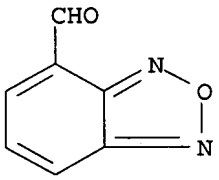
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-1-[(2-nitrophenyl)methyl]-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



IT 32863-32-4, 2,1,3-Benzoxadiazole-4-carboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of photoactivated calcium modulator prodrug)

RN 32863-32-4 CAPLUS

CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



L9 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:185276 CAPLUS

DOCUMENT NUMBER: 114:185276

TITLE: A process for preparation of enantiomerically pure polysubstituted 1,4-dihydropyridines

INVENTOR(S): Gandolfi, Carmelo A.; Frigerio, Marco; Riva, Carlo; Zaliani, Andrea; Long, Giorgio; Di Domenico, Roberto

PATENT ASSIGNEE(S): Boehringer Biochemia Robin S.p.A., Italy

SOURCE: Eur. Pat. Appl., 32 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

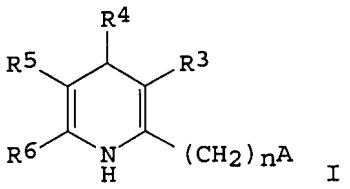
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 383320	A1	19900822	EP 1990-102951	19900215
R: GR				
CA 2047741	A1	19900818	CA 1990-2047741	19900215
WO 9009376	A1	19900823	WO 1990-EP243	19900215
W: AU, BB, BG, BR, CA, FI, HU, JP, KP, KR, LK, MC, MG, MW, NO, RO, SD, SU, US				
RW: AT, BE, BF, BJ, CF, CG, CH, CM, DE, DK, ES, FR, GA, GB, IT, LU, ML, MR, NL, SE, SN, TD, TG				
AU 9050904	A	19900905	AU 1990-50904	19900215
AU 630928	B2	19921112		
EP 458823	A1	19911204	EP 1990-903015	19900215
EP 458823	B1	19931013		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 04505610	T	19921001	JP 1990-503175	19900215
HU 62270	A2	19930428	HU 1990-1962	19900215
AT 95813	T	19931015	AT 1990-903015	19900215
ES 2060144	T3	19941116	ES 1990-903015	19900215
RU 2069658	C1	19961127	RU 1990-5001680	19900215
US 5245039	A	19930914	US 1991-743415	19910814
NO 9103188	A	19910815	NO 1991-3188	19910815
NO 177186	B	19950424		
NO 177186	C	19950802		
FI 95371	B	19951013	FI 1991-3861	19910815
FI 95371	C	19960125		

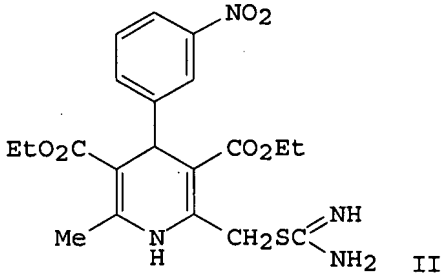
PRIORITY APPLN. INFO.:
IT 1989-19477 A 19890217
EP 1990-903015 A 19900215
WO 1990-EP243 A 19900215

OTHER SOURCE(S): MARPAT 114:185276

GI



I



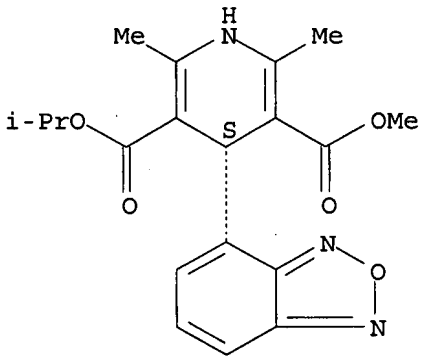
II

AB The title compds. [I; R3 = (esterified) CO2H; R4 = (substituted) Ph, β-naphthyl, heterocyclyl, etc.; R5 = cyano, NO2, (esterified) CO2H, etc.; R6 = C1-6 alkyl halo-C1-6-alkyl, HOC, CN, etc.; A = H, isothioureido, SH, sulfonium salt, etc.; n = 1-4], useful as cardiovascular agents (no data), are prepared A mixture of 6 g (±)-I (A = Cl, R3 = R5 = CO2Et, R4 = 3-O2NC6H4, R6 = Me, n = 1) and 1.2 g thiourea in EtOH was refluxed to give 4.8 g isothiuronium salt (±)-II.HCl, which was treated with NaHCO2 in EtOAc-H2O to give free (±)II. Optical resolution of (±)-II with O,O'-dibenzoyl-D-tartaric acid gave (+)-II of >98% optical purity. Also prepared were over 100 chiral I.

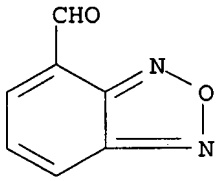
IT 84260-64-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cardiovascular agent)

RN 84260-64-0 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (4S)- (CA INDEX NAME)

Absolute stereochemistry.



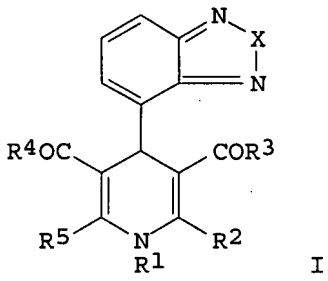
IT 32863-32-4, 4-Benzofurazancarboxaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with in preparation of cardiovascular agents)
RN 32863-32-4 CAPLUS
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



L9 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:94566 CAPLUS
DOCUMENT NUMBER: 108:94566
TITLE: Preparation of benzoxa- and benzothiadiazolecarboxaldehydes and their conversion to dihydropyridines
INVENTOR(S): Heitzmann, Markus
PATENT ASSIGNEE(S): Sandoz A.-G., Switz.
SOURCE: Patentschrift (Switz.), 4 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CH 661270	A5	19870715	CH 1982-6651		19821115
CH 661728	A5	19870814	CH 1982-1016		19821115
HU 44768	A2	19880428	HU 1986-1793		19860429
HU 196384	B	19881128			
DD 259400	A5	19880824	DD 1987-301996		19870421
PRIORITY APPLN. INFO.:			GB 1981-34708	A	19811118
			CH 1982-6651	A	19821115

OTHER SOURCE(S): CASREACT 108:94566
GI



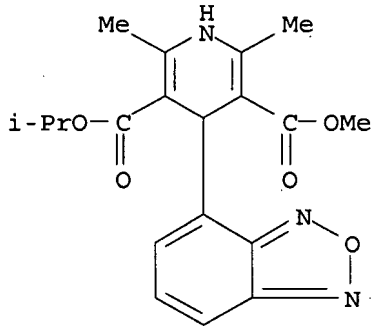
I

AB The title compds. [I; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) phenylalkyl; R2, R5 = H, alkyl; R3, R4 = alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, hydroxyalkoxy, alkenyloxy, etc; X = O, S] were prepared as drugs (no data). 2,1,3-Benzoxadiazole in THF was added to a solution of Li diisopropylamide in THF-cyclohexane at -75° and the resulting salt was added to DMF in THF. The initial adduct was hydrolyzed with aqueous HOAc and II was isolated via its bisulfite adduct. II was refluxed with Et acetoacetate and NH4OAc in EtOH to give I (R1 = H, R2 = R5 = Me, R3 = R4 = OEt).

IT 75695-93-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)

RN 75695-93-1 CAPLUS

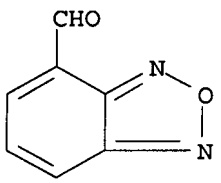
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)



IT 32863-32-4P, 2,1,3-Benzoxadiazole-4-carboxaldehyde
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as drug intermediate)

RN 32863-32-4 CAPLUS

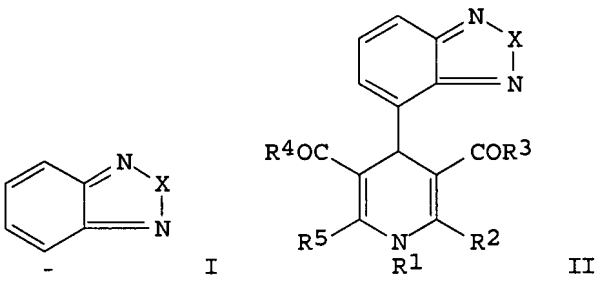
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



L9 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:636717 CAPLUS
DOCUMENT NUMBER: 107:236717
TITLE: Preparation of metallated 2,1,3-benzoxa-or -thiadiazole and their use in synthesis of dihydropyridine derivatives
INVENTOR(S): Heitzmann, Markus
PATENT ASSIGNEE(S): Sandoz A.-G., Switz.
SOURCE: Patentschrift (Switz.), 3 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 661728	A5	19870814	CH 1982-1016	19821115
CH 661270	A5	19870715	CH 1982-6651	19821115
PRIORITY APPLN. INFO.:			GB 1981-34708 A	19811118
			CH 1982-6651 A	19821115

GI

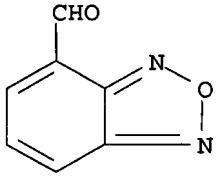


I II

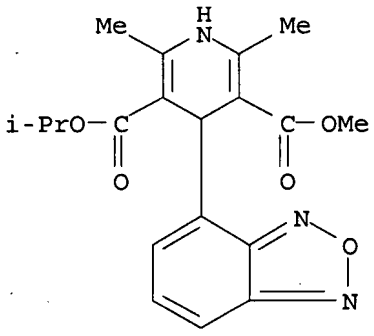
AB The title anions (I; X = O,S) were prepared by metalation of the parent heterocycles for use in synthesis of pharmacol. active dihydropyridines II [R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, (substituted) phenylalkyl; R2,R5 = H, alkyl; R3,R4 = alkyl, alkenyl, alkynyl, alkoxy, alkynyloxy, etc.]. 2,1,3-Benzoxadiazole in THF was added to a solution of LiN(CHMe2)2 in THF/cyclohexane at -78° and stirred for 35 min to afford the Li salt of I(X = O), which was added to DMF in THF followed by HOAc/H2O workup to give 2,1,3-benzoxadiazole-4-carboxaldehyde. The latter was cyclocondensed with MeCOCH2CO2Et and NH4OAc in EtOH to give II (R1 = H, R2 = R5 = Me, R3 = R4 = Et, X = O).

IT 32863-32-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with acetoacetate and ammonium acetate)

RN 32863-32-4 CAPLUS
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



IT 75695-93-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as drug)
RN 75695-93-1 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)

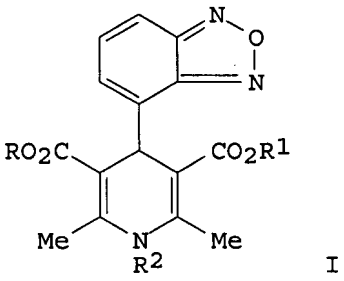


L9 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:407162 CAPLUS
DOCUMENT NUMBER: 101:7162
TITLE: 1,4-Dihydropyridine derivatives in optically active or in racemate form and their pharmaceutical compositions
INVENTOR(S): Vogel, Arnold
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.
SOURCE: Ger. Offen., 29 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3320616	A1	19831215	DE 1983-3320616	19830608
FR 2528431	A1	19831216	FR 1983-9551	19830607
FR 2528431	B1	19860110		
FI 8302072	A	19831216	FI 1983-2072	19830608
BE 897000	A1	19831209	BE 1983-10806	19830609
NL 8302067	A	19840102	NL 1983-2067	19830610
WO 8400033	A1	19840105	WO 1983-CH73	19830610
W: CH				
CH 660593	A5	19870515	CH 1984-688	19830610
DK 8302711	A	19831216	DK 1983-2711	19830613
GB 2122192	A	19840111	GB 1983-16054	19830613
GB 2122192	B	19851218		
CA 1208639	A1	19860729	CA 1983-430300	19830613
IL 68975	A	19870130	IL 1983-68975	19830613
SE 8303385	A	19831216	SE 1983-3385	19830614
AU 8315753	A	19831222	AU 1983-15753	19830614
JP 59005183	A	19840112	JP 1983-106597	19830614
HU 33802	A2	19841228	HU 1983-2113	19830614
HU 191853	B	19870428		
ES 523243	A1	19850401	ES 1983-523243	19830614
AT 8302183	A	19870315	AT 1983-2183	19830614
AT 384219	B	19871012		

ZA 8304409	A	19850227	ZA 1983-4409		19830615
ES 538157	A1	19860201	ES 1984-538157		19841130
PRIORITY APPLN. INFO.:			CH 1982-3692	A	19820615
			CH 1982-3693	A	19820615
			WO 1983-CH73	A	19830610

OTHER SOURCE(S): MARPAT 101:7162
GI



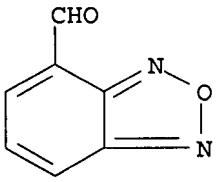
I

AB Calcium channel blocking (no data) benzoxadiazolylpyridinedicarboxylates I [1 of R,R1 = Me, the other = Me2CH, Bu, Me2CHCH2, Me2CHOCH2CH2, cyclopentyl; R2 = (un)substituted C1-6 alkyl] were prepared Thus, I (R = Me, R1 = Me2CH, R2 = H) was treated with (MeO)2SO2 in Me2SO to give (±)-I (R = Me, R1 = Me2CH, R2 = Me).

IT 32863-32-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with acetoacetate derivative)

RN 32863-32-4 CAPLUS

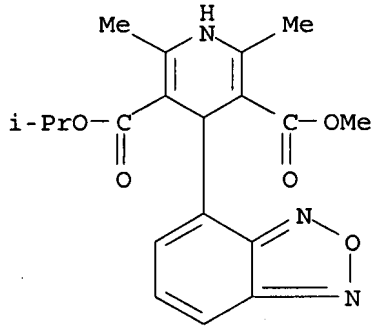
CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



IT 75695-93-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)

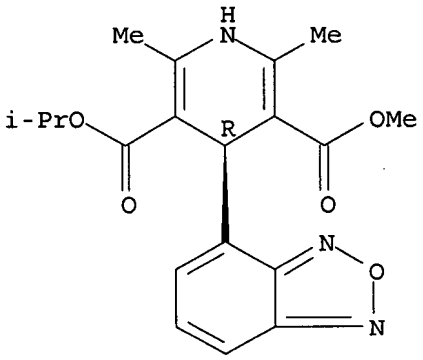
RN 75695-93-1 CAPLUS

CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)



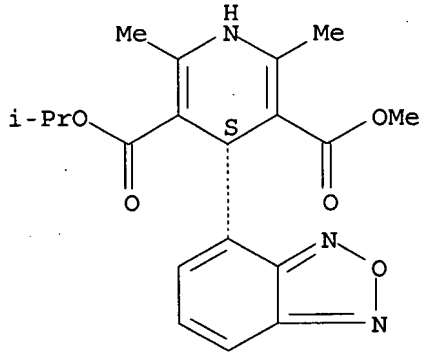
IT 84260-63-9P 84260-64-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 84260-63-9 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

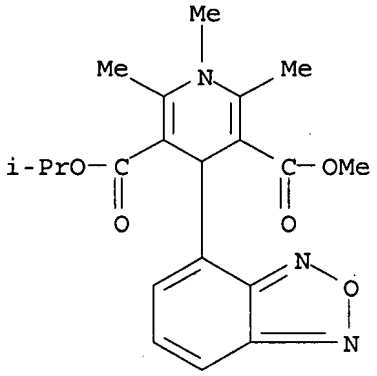


RN 84260-64-0 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (4S)- (CA INDEX NAME)

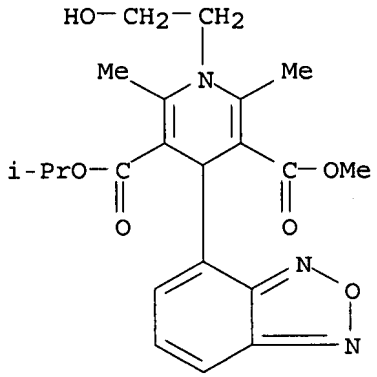
Absolute stereochemistry.



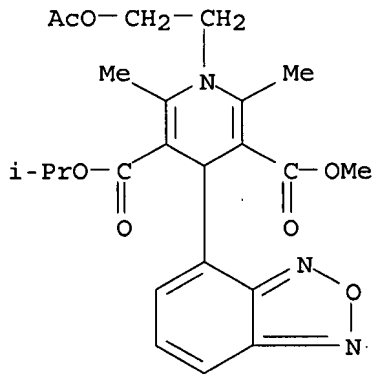
IT 88977-21-3P 88977-39-3P 88977-40-6P
88977-41-7P 88977-42-8P 88977-44-0P
88977-45-1P 88977-46-2P 88987-07-9P
88987-08-0P 88987-09-1P 89016-38-6P
89016-39-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 88977-21-3 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-1,2,6-trimethyl-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



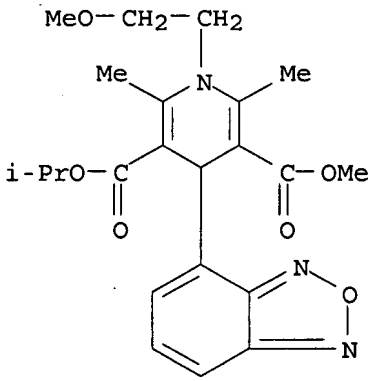
RN 88977-39-3 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-1-(2-hydroxyethyl)-2,6-dimethyl-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



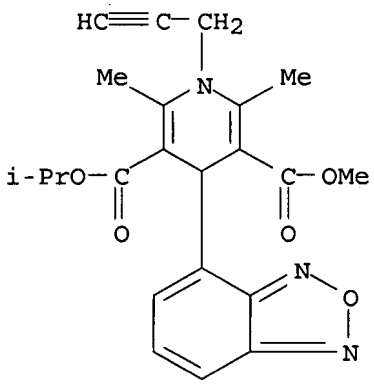
RN 88977-40-6 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 1-[2-(acetyloxy)ethyl]-4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 88977-41-7 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-1-(2-methoxyethyl)-2,6-dimethyl-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



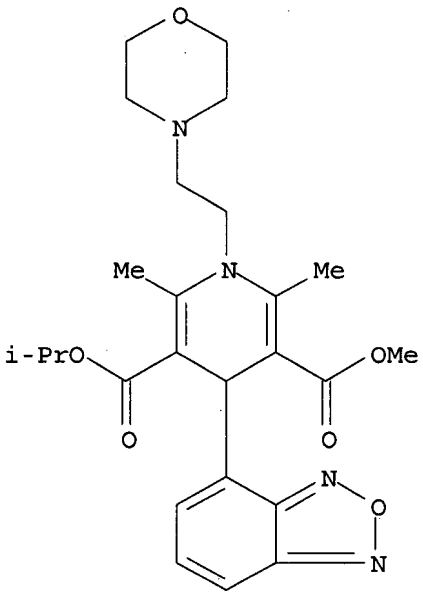
RN 88977-42-8 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-1-(2-propynyl)-, methyl 1-methylethyl ester (9CI) (CA INDEX NAME)



RN 88977-44-0 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-1-[2-(4-morpholinyl)ethyl]-, methyl 1-methylethyl ester, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

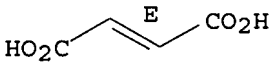
CRN 88977-43-9
CMF C25 H32 N4 O6



CM 2

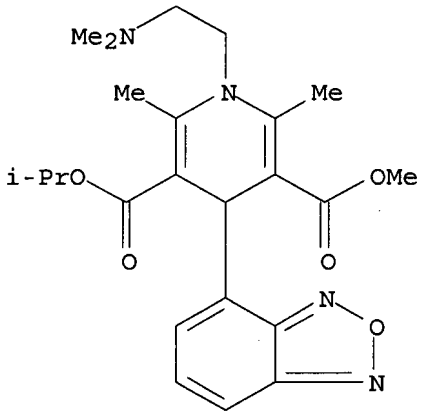
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



RN 88977-45-1 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1-[2-(dimethylamino)ethyl]-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (-)- (9CI) (CA INDEX NAME)

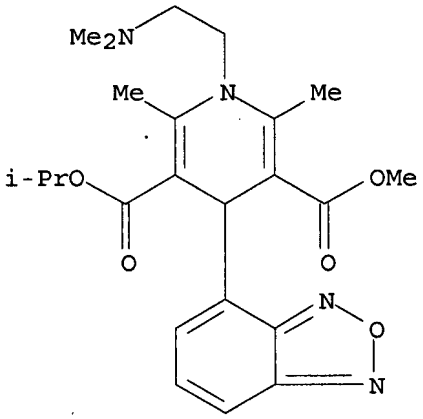
Rotation (-).



RN 88977-46-2 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1-[2-(dimethylamino)ethyl]-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl

ester, hydrobromide, (-)- (9CI) (CA INDEX NAME)

Rotation (-).

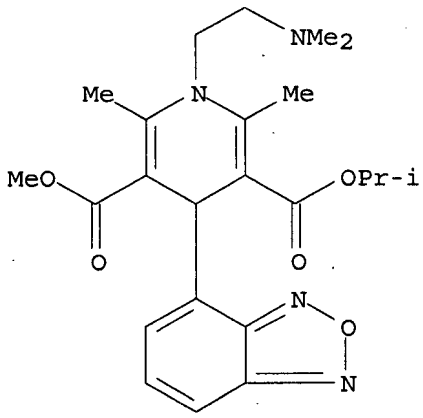


●x HBr

RN 88987-07-9 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1-[2-(dimethylamino)ethyl]-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

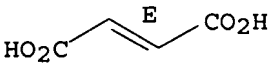
CRN 88987-06-8
CMF C23 H30 N4 O5



CM 2

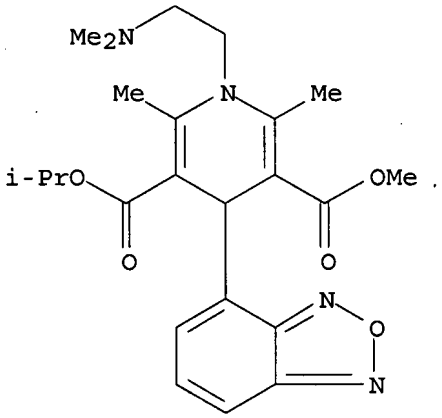
CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



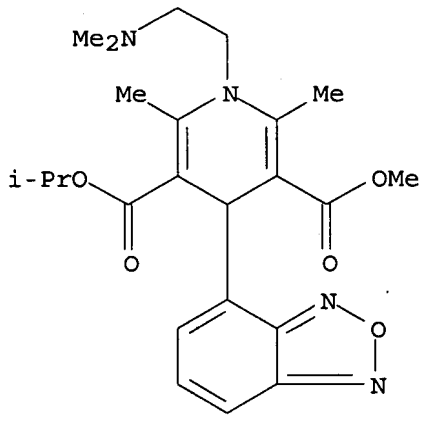
RN 88987-08-0 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1-[2-(dimethylamino)ethyl]-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, (+)- (9CI) (CA INDEX NAME)

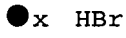
Rotation (+).



RN 88987-09-1 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1-[2-(dimethylamino)ethyl]-1,4-dihydro-2,6-dimethyl-, methyl 1-methylethyl ester, hydrobromide, (+)- (9CI) (CA INDEX NAME)

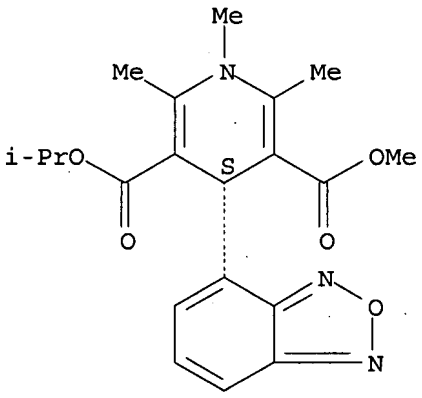
Rotation (+).





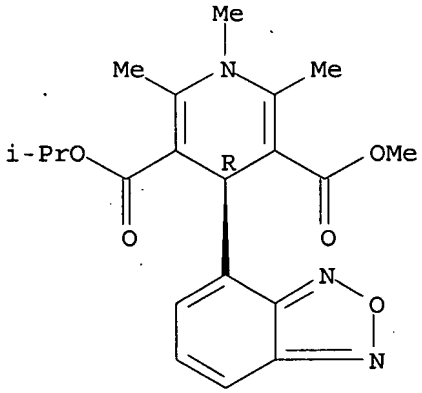
RN 89016-38-6 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-1,2,6-trimethyl-, methyl 1-methylethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 89016-39-7 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-1,2,6-trimethyl-, methyl 1-methylethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L9 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:639420 CAPLUS
DOCUMENT NUMBER: 93:239420
TITLE: 1,4-Dihydropyridines and their use
INVENTOR(S): Neumann, Peter
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Switz.
SOURCE: Ger. Offen., 12 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2949491	A1	19800626	DE 1979-2949491	19791208
DE 2949491	C2	19881027		
CH 639659	A5	19831130	CH 1978-12835	19781218
SE 7910188	A	19800619	SE 1979-10188	19791211
SE 445219	B	19860609		
SE 445219	C	19860918		
BE 880591	A1	19800613	BE 1979-9643	19791213
NL 7909024	A	19800620	NL 1979-9024	19791214
NL 193066	B	19980506		

NL 193066	C	19980908			
GB 2037766	A	19800716	GB 1979-43113		19791214
GB 2037766	B	19830216			
JP 55083783	A	19800624	JP 1979-163965		19791217
JP 03069910	B	19911105			
AU 7953896	A	19800626	AU 1979-53896		19791217
AU 536055	B2	19840419			
FR 2444681	A1	19800718	FR 1979-30829		19791217
FR 2444681	B1	19821029			
ZA 7906842	A	19810729	ZA 1979-6842		19791218
CH 654836	A5	19860314	CH 1980-5484		19800717
AU 536069	B2	19840419	AU 1982-79464		19820112
AU 8279464	A	19820408			
US 4466972	A	19840821	US 1982-359751		19820319
GB 2103203	A	19830216	GB 1982-15988		19820601
GB 2103203	B	19830608			

PRIORITY APPLN. INFO.:

CH 1978-12835	A	19781218
CH 1977-7520	A	19770620
CH 1978-2865	A	19780316
US 1978-915858	A2	19780615
CH 1978-12888	A	19781218
CH 1978-12890	A	19781218
CH 1979-3472	A	19790411
CH 1979-3477	A	19790411
CH 1979-5627	A	19790615
GB 1979-40624		19791123
DE 1979-2949491	A	19791208
US 1979-101591	A2	19791210
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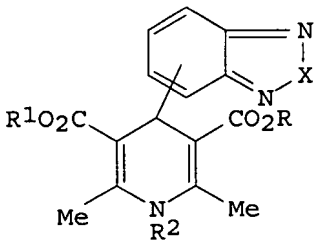
US 1980-173305	A1	19800729

GI



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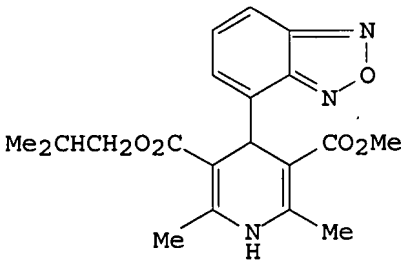


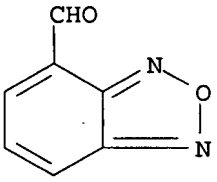
II

AB Dihydropyridines I (R = C1-4 alkyl, alkoxyalkyl, cyclopentyl; R1 = C1-4 alkyl; R2 = H, Me, Pr; X = O, S) were prepared for use as vasodilators, antihypertensives, Ca antagonists, and in the treatment of angina pectoris (no data). Thus 2,1,3-benzoxadiazole-4-carboxaldehyde was condensed with AcCH2CO2CH2CHMe2 and H2NCMe:CHCO2Me to give II.

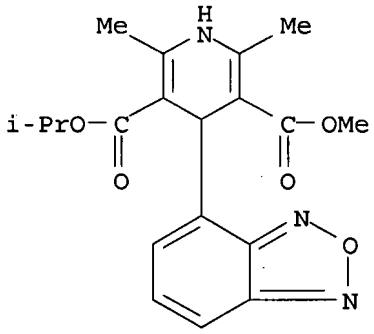
IT 32863-32-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with acetoacetate and aminocrotonate)

RN 32863-32-4 CAPLUS

CN 2,1,3-Benzoxadiazole-4-carboxaldehyde (CA INDEX NAME)



IT 75695-93-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 75695-93-1 CAPLUS
CN 3,5-Pyridinedicarboxylic acid, 4-(2,1,3-benzoxadiazol-4-yl)-1,4-dihydro-2,6-dimethyl-, 3-methyl 5-(1-methylethyl) ester (CA INDEX NAME)



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